Supporting Information for the manuscript *"Simulations on the Thermal Decomposition of a Polydimethylsiloxane Polymer Using the ReaxFF Reactive Force Field"* by Kimberly Chenoweth, Sam Cheung, Adri C.T. van Duin, Edward M. Kober and William A. Goddard III.

ReaxFF force field parameter file:

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Reactive MD-force field
 39       ! Number of general parameters
   50.0000 !Overcoordination parameter
    9.5469 !Overcoordination parameter
   26.5405 !Valency angle conjugation parameter
    3.0000 !Triple bond stabilisation parameter
    6.5000 !Triple bond stabilisation parameter
    0.0000 !C2-correction
    1.0588 !Undercoordination parameter
    9.0000 !Triple bond stabilisation parameter
   12.1176 !Undercoordination parameter
   13.3056 !Undercoordination parameter
    0.0000 !Triple bond stabilization energy
    0.0000 !Lower Taper-radius
   10.0000 !Upper Taper-radius
    2.8793 !Not used
   33.8667 !Valency undercoordination
    6.0891 !Valency angle/lone pair parameter
    1.0563 !Valency angle
    2.0384 !Valency angle parameter
    6.1431 !Not used
    6.9290 !Double bond/angle parameter
    0.3989 !Double bond/angle parameter: overcoord
    3.9954 !Double bond/angle parameter: overcoord
   -2.4837 !Not used
    5.7796 !Torsion/BO parameter
   10.0000 !Torsion overcoordination
    1.9487 !Torsion overcoordination
   -1.2327 !Conjugation 0 (not used)
    2.1645 !Conjugation
    1.5591 !vdWaals shielding
    0.0100 !Cutoff for bond order (*100)
    2.1365 !Valency angle conjugation parameter
    1.5001 !Overcoordination parameter
    3.2593 !Overcoordination parameter
    1.8512 !Valency/lone pair parameter
    0.5000 !Not used
   20.0000 !Not used
    5.0000 !Molecular energy (not used)
    0.0000 !Molecular energy (not used)
    2.6962 !Valency angle conjugation parameter
  5    ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
            alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
            cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
            ov/un;val1;n.u.;val3,vval4
 C     1.3644   4.0000  12.0000   1.9803   0.1720   0.8712   1.2395   4.0000
       9.4734   2.1241   4.0000  31.8793  79.5548   5.7254   6.9235   0.0000
       1.2636   0.0000  -0.0537   5.7133  33.5629  11.9957   0.8563   0.0000
      -2.8983   4.7820   1.0564   4.0000   2.9663   0.0000   0.0000   0.0000
 H     0.6853   1.0000   1.0080   1.3588   0.0622   0.7625  -0.1000   1.0000
       9.3992   5.0518   1.0000   0.0000 121.1250   3.8196   9.8832   1.0000
      -0.1000   0.0000  -0.1609   3.8654   3.2462   1.0000   1.0698   0.0000
     -15.7683   3.3504   1.0338   1.0000   2.8793   0.0000   0.0000   0.0000
 O     1.2891   2.0000  15.9990   1.9741   0.0880   0.8628   1.0323   6.0000
      10.2186   7.7719   4.0000  30.8697 116.0768   8.5000   6.9793   2.0000
       0.9456  29.2540  -1.3533  20.7724   3.5512   0.5074   0.9745   0.0000
      -3.6141   2.7025   1.0493   4.0000   2.9225   0.0000   0.0000   0.0000
 Si    1.9007   4.0000  28.0600   1.9947   0.2201   0.6294   1.2962   4.0000
      12.9535   1.3506   4.0000  24.9985 139.9309   2.9154   7.0174   0.0000
      -1.0000   0.0000 128.2031   4.6110 190.1166   0.8381   0.8563   0.0000
      -5.4765   2.2852   1.0338   4.0000   2.5791   0.0000   0.0000   0.0000
```

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X   -0.1000   2.0000   1.0080   2.0000   0.0000   1.0000  -0.1000   6.0000
    10.0000   2.5000   4.0000   0.0000   0.0000   8.5000   1.5000   0.0000
    -0.1000   0.0000 127.6226   8.7410  13.3640   0.6690   0.9745   0.0000
   -11.0000   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
10      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                       pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
 1  1 139.8093 110.6913  77.2102   0.2737  -0.7584   1.0000  38.4226   0.3288
       0.1235  -0.2010   8.6973   1.0000  -0.1042   6.1688   1.0000   0.0000
 1  2 159.8520   0.0000   0.0000  -0.4646   0.0000   1.0000   6.0000   0.6170
      12.3878   1.0000   0.0000   1.0000  -0.0098   8.5954   0.0000   0.0000
 2  2 170.0433   0.0000   0.0000  -0.3573   0.0000   1.0000   6.0000   0.7489
       9.6471   1.0000   0.0000   1.0000  -0.0169   5.8818   0.0000   0.0000
 1  3 161.6647  58.4169 126.5609   0.2952  -0.1638   1.0000  12.1551   0.4055
       0.3211  -0.2388   7.5568   1.0000  -0.1729   4.9857   0.0000   0.0000
 3  3  87.8137 171.0665  40.0000   0.9810  -0.2106   1.0000  29.4721   1.0000
       0.8827  -0.1679   7.7980   1.0000  -0.1290   7.0000   1.0000   0.0000
 1  4 119.1620  83.3504   0.0000   0.1175  -0.5558   1.0000  17.2117   0.1009
       0.2527  -0.2869   8.3842   1.0000  -0.1064   6.4957   1.0000   0.0000
 2  4 261.8327   0.0000   0.0000  -0.7842   0.0000   1.0000   6.0000   0.5715
      20.0570  -0.0103   0.0000   1.0000  -0.0474   6.5704   0.0000   0.0000
 3  4 282.1448  39.0786   0.0000  -0.8744  -0.3000   1.0000  36.0000   0.5909
       9.4685  -0.4537  30.3000   1.0000  -0.1142   6.9349   1.0000   0.0000
 4  4  86.6074  47.8910  30.0000   0.6601  -0.3000   1.0000  16.0000   0.0145
       0.3370  -0.1786  18.1800   1.0000  -0.0593   8.0170   0.0000   0.0000
 7    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
 1  2   0.0431   1.7204  10.3632   1.0386  -1.0000  -1.0000
 1  3   0.1142   1.9602   9.4709   1.3065   1.1260   1.0865
 2  3   0.0450   1.8703  10.4434   0.9232  -1.0000  -1.0000
 1  4   0.0529   2.0696  13.2006   1.7495   1.5081  -1.0000
 2  4   0.0659   1.4966  13.7160   1.3115  -1.0055  -1.0000
 3  4   0.1156   2.0255  11.3726   1.7205   1.3699  -1.0000
 4  4   0.1365   1.9123  11.1784   1.7095   1.4858  -1.0000
40    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2;val(bo)
 1  1  1  75.3892  20.0233   2.1017   2.4996   0.0031  35.9933   1.0400
 1  1  2  71.5185  11.6939   6.5331   0.0000   0.0000   0.0000   1.0400
 2  1  2  72.0977   8.3496   2.2003   0.0000   0.2000   0.0000   1.0400
 1  2  2   0.0000   0.0000   6.0000   0.0000   0.0000   0.0000   1.0400
 1  2  1   0.0000  28.5244   6.0000   0.0000   0.0000   0.0000   1.0400
 2  2  2   0.0000  27.9213   5.8635   0.0000   0.0000   0.0000   1.0400
 1  1  3  74.0268  28.8967   1.2260   0.0000   4.6228   0.0000   1.0400
 3  1  3  80.2138  52.6408   1.3212   0.0000   4.6228 -35.0000   1.0400
 2  1  3  79.3704  19.7034   2.5917   0.0000   0.0000   0.0000   1.0400
 1  3  1  76.4435  43.0224   0.6138   0.0000   0.4897   0.0000   1.0400
 1  3  3  81.4803  53.9823   0.8786   0.0000   0.4897   0.0000   1.0400
 3  3  3  78.4963  61.0192   1.0093 -38.4200   0.4897   0.0000   1.0400
 1  3  2  82.1464  36.8788   1.3932   0.0000   0.0000   0.0000   1.0400
 2  3  3  89.4640  10.1026   4.7764   0.0000   0.0000   0.0000   1.0400
 2  3  2  81.7479  15.4269   4.2247   0.0000   0.0000   0.0000   1.0400
 1  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 3  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 2  2  3   0.0000   0.0019   6.0000   0.0000   0.0000   0.0000   1.0400
 4  4  4  78.5354  38.9251   0.8265   0.0000   0.0100   0.0000   1.2887
 2  4  4  79.0822  11.1429   2.5009   0.0000   2.7527   0.0000   1.2359
 2  4  2  79.0377   9.4230   4.0267   0.0000   3.2371   0.0000   1.0050
 3  4  4  75.1800  19.3598   1.2213   0.0000   3.9834   0.0000   1.1463
 2  4  3  63.9892  16.5864   4.1343   0.0000   3.2120   0.0000   1.0000
 3  4  3  89.0000  34.7562   0.3372   0.0000   0.2152   0.0000   1.2711
 4  3  4  63.5212   1.7624   0.3862   0.0000   2.6557   0.0000   1.1252
 2  3  4  69.2579   4.4688   5.8970   0.0000   3.6100   0.0000   1.1218
 3  3  4  87.1521  16.3509   2.2547   0.0000   1.1312   0.0000   1.0758
 2  2  4   0.0000  49.9658   5.9898   0.0000   1.6112   0.0000   1.0279
 4  2  4   0.0000  24.8597   5.8973   0.0000   1.5840   0.0000   1.0634
 3  2  4   0.0000   7.4792   3.9744   0.0000   1.6980   0.0000   1.0099
 1  1  4  64.5561  20.9500   1.9842   0.0000   1.0417   0.0000   1.0477
 1  4  1  69.6070  20.4933   2.1373   0.0000   1.0375   0.0000   1.1315
 4  1  4  58.7586  16.6923   1.9877   0.0000   0.9878   0.0000   1.0094
 1  4  4  71.3550  20.3460   2.0415   0.0000   1.0111   0.0000   1.0345
 2  1  4  67.2572  11.8513   2.4212   0.0000   1.0191   0.0000   1.0202
 1  4  2  71.0461  15.3115   2.4106   0.0000   1.0505   0.0000   1.1311
 1  3  4  83.4540  13.2996   0.9157   0.0000   0.9692   0.0000   1.2768
 1  4  3  60.1831  41.2192   1.3565   0.0000   1.0285   0.0000   1.0135
 3  1  4  76.6122   5.4827   0.9914   0.0000   0.9836   0.0000   1.2774
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 1   2   4    0.0000    2.7081    1.1497    0.0000    0.9548    0.0000    1.2657
13      ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
 1   1   1   1    0.0000   38.9174    0.3649   -8.2931   -2.0127    0.0000    0.0000
 1   1   1   2    0.0000   49.1001    0.2713   -8.5284   -1.5309    0.0000    0.0000
 2   1   1   2    0.0000   34.0265    0.3804   -6.3917   -0.9965    0.0000    0.0000
 0   1   2   0    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000
 0   2   2   0    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000
 0   1   3   0    3.9830   13.0320    0.4739   -1.9813   -2.0000    0.0000    0.0000
 0   2   3   0    0.0000    0.1000    0.0200   -2.5415    0.0000    0.0000    0.0000
 0   3   3   0    0.0318   23.1045    1.2614  -12.3670    0.0000    0.0000    0.0000
 0   1   1   0    0.0000    0.6675    0.0000   -8.2352    0.0000    0.0000    0.0000
 2   4   4   2    0.0000    0.0000    0.0640   -2.4426    0.0000    0.0000    0.0000
 2   4   4   4    0.0000    0.0000    0.1587   -2.4426    0.0000    0.0000    0.0000
 0   2   4   0    0.0000    0.0000    0.1200   -2.4847    0.0000    0.0000    0.0000
 6   3   4   1    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000    0.0000
 1      ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
 3   2   3    2.2017   -7.1638    1.6003    1.7032
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Figure 1. Comparison of ReaxFF and QC energies for Si-C single bond in $H_3Si\text{-}CH_3$.

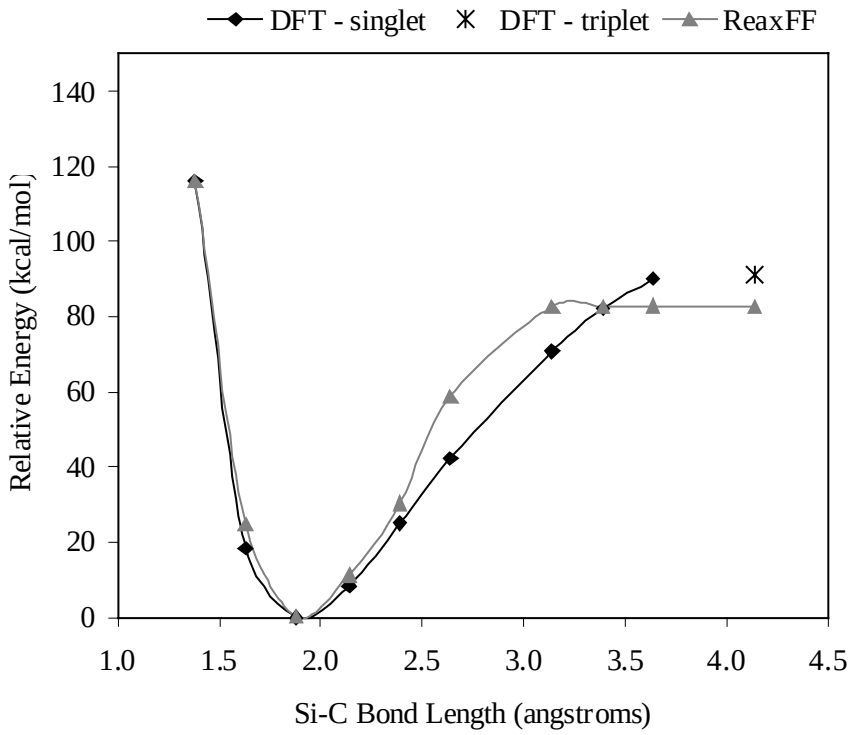

Figure 2. ReaxFF and QC distortion energies for the C-C-Si (a), C-Si-C (b), Si-Si-C (c), Si-C-Si (d), Si-C-H (e), C-Si-H (f).